```
chain nodes :
7 9 12
ring nodes :
1 2 3 4 5 11
chain bonds :
3-7 7-9 9-12
ring bonds :
1-2 1-5 1-11 2-3 2-11 3-4 3-11 4-5 4-11 5-11
exact/norm bonds :
1-2 1-5 1-11 2-3 2-11 3-4 3-7 3-11 4-5 4-11 5-11 7-9 9-12
G1:C,Si,Ge
G2:O,S,N,P,As,Sb,Se,Te
G3:Cr,Mo,W
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:CLASS 11:Atom 12:Atom
L1 STRUCTURE UPLOADED
=> d his
    (FILE 'HOME' ENTERED AT 11:06:01 ON 11 MAY 2009)
    FILE 'REGISTRY' ENTERED AT 11:07:19 ON 11 MAY 2009
L1
              STRUCTURE UPLOADED
=> d 11
L1 HAS NO ANSWERS
L1
              STR
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G2 O, S, N, P, As, Sb, Se, Te

G3 Cr, Mo, W

Structure attributes must be viewed using STN Express query preparation.

=> s 11 full FULL SEARCH INITIATED 11:08:02 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 61481 TO ITERATE

100.0% PROCESSED 61481 ITERATIONS SEARCH TIME: 00.00.02 18 ANSWERS

L2 18 SEA SSS FUL L1

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FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 185.88 186.32

FILE 'CAPLUS' ENTERED AT 11:08:12 ON 11 MAY 2009
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FILE COVERS 1907 - 11 May 2009 VOL 150 ISS 20
FILE LAST UPDATED: 8 May 2009 (2009508/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate

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=> s 12
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8 L2

=> d 1-8 bib abs

- ANSWER 1 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:1463161 CAPLUS
- DN 148:285296
- ΤТ Syntheses and spectra of chromium-titanium complexes bridged by carboxylate substituted cyclopentadienyl group: The structure of Cp2Ti(CH3) { [OC(O)C5H4]Cr(NO)2C1}
- ΑU Wang, Yu-Pin; Pang, Su-Ru; Cheng, Hsiu-Yao; Lin, Tso-Shen; Wang, Yu; Lee, Gene-Hsiang
- CS Department of Chemistry, Tunghai University, Taichung, Taichung, Taiwan Journal of Organometallic Chemistry (2008), 693(2), 329-337 SO CODEN: JORCAI; ISSN: 0022-328X
- PB Elsevier Ltd.
- DT Journal
- LA English
- CASREACT 148:285296 OS
- Mono-demethylation of Cp2Ti(CH3)2 in dichloromethane with 1 M equivalent of [n5-(C5H4COOH)]Cr(CO)2NO(5), [n5-(C5H4COOH)]Cr(NO)2X(X = C1.6, X)= I 7) and [η5-(C5H4COOH)]W(CO)3CH3 (8) gives

Cp2Ti(CH3) { [OC(0)C5H4]Cr(CO)2NO} (9), Cp2Ti(CH3) { [OC(0)C5H4]Cr(NO)2C1} (10), Cp2Ti(CH3){[OC(O)C5H4]Cr(NO)2I} (11), and

Cp2Ti(CH3) { [OC(O)C5H4] W(CO)3CH3} (12), resp. The structure of 10 has been solved by x-ray diffraction studies. One of the nitrosyl groups is located at the site away from the exocyclic carbonyl carbon of the Cp(Cr)

ring with twist angle of 178.1°. All the data reveals that Cp2Ti(CH3)- is a strong electron-donating group. The opposite correlation was observed on the chemical shift assignments of C(2)-C(5) in compds. 5-12, using HetCOR NMR spectroscopy, as compared with the NMR data of their

ferrocene analogs. The electron d. distribution in the cyclopentadienyl ring is discussed on the basis of 13C NMR data and those of 10 are compared with the calcus, via d. functional B3LYP correlation-exchange method.

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- 1.3 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2001:527829 CAPLUS
- 135:253344 DN
- ΤI Photoinduced DNA Cleavage by Cyclopentadienyl Metal Complexes Conjugated to DNA Recognition Elements
- Hurley, Allison L.; Maddox, Mitchell P., III; Scott, Tricia L.; Flood, ΑU Mark R.; Mohler, Debra L. Department of Chemistry, Emory University, Atlanta, GA, 30322, USA Organic Letters (2001), 3(17), 2761-2764 CODEN: ORLEF7; ISSN: 1523-7060
- CS
- SO
- American Chemical Society PB
- Journal
- T.A English
- OS CASREACT 135:253344
- DNA recognition elements have been attached to CpW(CO)3CH3 and CpW(CO)3Ph, AR which produce Me and Ph radicals that cleave DNA upon photolysis. The inclusion of binding moieties in 3 increases the efficiency but not the

selectivity of strand scission over that seen in the simple unfunctionalized complex, while 11 cleaves preferentially at T sites within AT-rich tracts.

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- ANSWER 3 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2000:556554 CAPLUS
- DN 134:38379
- TI Organometallic Photonucleases: Synthesis and DNA-Cleavage Studies of Cyclopentadienyl Metal-Substituted Dendrimers Designed To Increase Double-Strand Scission
- ΑU Hurley, Allison L.; Mohler, Debra L.
- CS Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
- SO. Organic Letters (2000), 2(18), 2745-2748 CODEN: ORLEF7; ISSN: 1523-7060
- American Chemical Society PR
- DT Journal
- LA English
- os CASREACT 134:38379
- AB A series of metal complex-substituted polyamine dendrimers have been synthesized and examined for their ability to cleave plasmid DNA in a double-stranded manner. While photolysis of the dimetallic spermine derivative and the tetrametallic DAB-Am-4 complex led to double-strand scission, in the larger DAB-Am-8 and DAB-Am-16 systems, DNA
- aggregation/precipitation was the predominant competing process observed THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- 1.3 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 1997:383367 CAPLUS
- DN 127:121814
- OREF 127:23501a,23504a
- The synthesis and characterization of Group IV metal-chromium complexes bridged by an OCH2C5H4 group. The molecular structure of Cp2TiCl[(OCH2C5H4)Cr(CO)2(NO)]
- AU Jiang, Ming-Ke; Lin, Chu-Chieh; Gau, Han-Mou

energies of v(CO) and v(NO) bands.

- CS Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan
- SO Journal of Organometallic Chemistry (1997), 539(1-2), 155-161 CODEN: JORCAI; ISSN: 0022-328X
- PB Elsevier
- DT Journal
- LA
- English AB The series of complexes  $Cp2TiY[(\mu-OCH2C5H4)Cr(CO)2(NO)]$  (Y = C1 (1), Br (2), or CH3 (3)) and Cp2ZrY[( $\mu$ -OCH2C5H4)Cr(CO)2(NO)] (Y = CH2Ph (4) or (µ-OCH2C5H4)Cr(CO)2(NO) (5)) were prepared from the reactions of (HOCH2C5H4)Cr(CO)2(NO) with suitable Group IV metallocene derivs. The IR spectra of complexes 1-5 show that the v(CO) and v(NO) shift to lower frequencies relative to the values for (HOCH2C5H4)Cr(CO)2(NO). This observation indicates more w-backbonding from the chromium metal center to the two CO and the NO ligands upon complexation of (OCH2C5H4)Cr(CO)2(NO) to the early metal. Complex 1 crystallizes in the monoclinic P21/n space group with cell parameters a = 11.274(2) Å, b =13.135(3) Å, c = 13.091(3) Å,  $\beta$  = 105.46(3)°, z = 4, R = 0.045, Rw = 0.054 and Gof = 1.23. The slightly long C-O and N-O distances, the considerably weak Ti-O bond and the upfield shift of the 1H and 13C chemical shifts of C5H4 group also support the argument of net electron flow from OCH2 group to C5H4 group in which the cumulated electron d. would pass to the chromium metal center and then

w-backbonding to the CO and NO ligands for the observation of lower

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD

## ALL CITATIONS AVAILABLE IN THE RE FORMAT

- ANSWER 5 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN L.3
- 1995:993310 CAPLUS AN
- DN 124:146389
- OREF 124:27237a,27240a
- Covalent and Selective Labeling of Proteins with Heavy Metals. Synthesis, x-ray Structure, and Reactivity Studies of N-Succinimidyl and N-Sulfosuccinimidyl Ester Organotungsten Complexes
- ΑU Gorfti, Abdelaziz; Salmain, Michele; Jaouen, Gerard; McGlinchev, Michael J.; Bennouna, Abdelaziz; Mousser, Abdelhamid
- CS Ecole Nationale Superieure de Chimie de Paris, CNRS, Paris, F-75231, Fr. SO Organometallics (1996), 15(1), 142-51
- CODEN: ORGND7; ISSN: 0276-7333 PB American Chemical Society
- DТ Journal
- LA English
- os CASREACT 124:146389
- GI

AΒ



- ONHR2 т
- (η1-enolate) W complexes bearing an N-succinimidyl or an N-sulfosuccinimidyl ester were prepared and fully characterized. The mol. structures of [n5-((succinimidooxy)carbonyl)cyclopentadienyl]methyltri carbonyltungsten(II) (2) and [η5-((succinimidooxy)carbonyl)cyclopentadienyl]iodotricarbonyltungsten(II) (5) were solved by x-ray crystallog. The reactivity of these activated esters, I (R = Me, I; R1 = H, S03-) toward a range of amines and amino acids was studied. While the N-succinimidyl ester enolate is unreactive, N-succinimidyl-substituted cyclopentadienyl complexes were quite reactive, leading to the expected stable organometallic amides II (R = Me, I; R2 = CH2Ph, CH2CH2CO2H). Bovine serum albumin (BSA), a 66 kDa mol. mass globular protein, could be labeled with fair yields, and conjugates were characterized by IR spectroscopy of the CO ligands. Organotungsten N-succinimidyl esters thus appear as promising reagents for the labeling

New functionally substituted  $\eta5$ -cyclopentadienyl and 2-oxaallyl

- ANSWER 6 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 1995:643155 CAPLUS
- DN 123:169812

ΑU

- OREF 123:30334h,30335a
- Comparative Study of the Structures and Reactivity of the
  - π-Cyclopentadienyl-Bonded and Metal-Bonded Succinimidyl Ester Complexes (Metal = Mo, Fe): X-ray Molecular Structures of

El Mouatassim, Bouchra; Elamouri, Hani; Vaissermann, Jacqueline; Jaouen,

- $[(\eta 5-C5H4COONS)Mo(CO)3Me]$  and  $[(\eta 5-C5H5)Mo(CO)3(\eta 1-CH2COONS)]$ (-NS = -N-Succinimidy1)
- Gerard Ecole Nationale Superieure de Chimie de Paris, Paris, 75231, Fr.
- Organometallics (1995), 14(7), 3296-302 SO

of proteins with heavy metals.

CODEN: ORGND7; ISSN: 0276-7333

PB American Chemical Society DT

Journal LA English

AB

OS CASREACT 123:169812

> The activated ester compds. [(n5-C5H4COONS)Mo(CO)3Me] (5) and [(n5-C5H4COONS)Fe(CO)2Me] (6) were obtained by treatment of the novel organometallic carboxylic acid complexes [(n5-C5H4COOH)Mo(CO)3Me] (2) and [(n5-C5H4COOH)Fe(CO)2Me] (4) with N-hydroxysuccinimide in THF in the presence of DCC (dicyclohexylcarbodiimide) or with DSC (disyccinimidyl carbonate) in CH3CN in the presence of pyridine. These activated ester complexes were identified spectroscopically, and in addition, the x-ray mol. structure of 5 was determined Compound 5 crystallizes in the triclinic space group P-1: a = 8.684(4) Å, b = 12.764(8) Å, c = 16.522(10) Å,  $\alpha = 65.13(4)^{\circ}$ ,  $\beta = 72.52(4)^{\circ}$ ,  $\gamma =$  $71.34(4)^{\circ}$ , V = 1544.6 Å3, Z = 4. Similarly, the metal-activated ester complex [(η5-C5H5)Mo(CO)3(η1-CH2COONS)] (7) was obtained by treatment of the dimer [Cp2Mo2(CO)6] with Na/Hg followed by addition of 2 equiv of C1CH2COONS in THF; in this compound the ester unit is bonded directly to the metal center rather than to the  $\pi$ -bonded cyclopentadienyl. Complex 7 was characterized by spectroscopic methods, and its mol. structure was ascertained by x-ray crystallog, which showed that it belongs to the well-known carbon-bound molvbdenum 2-oxaalkvl (n1-enolate) category. Complex 7 crystallizes in the monoclinic space group C2/c: a = 19.484(2) Å, b = 11.393(2) Å, c = 13.694(2) Å,

 $\beta = 98.91(2)^{\circ}$ , V = 3000 Å3, Z = 8. The reactivity of  $\pi$ -bonded activated ester complexes 5 and 6 with ISiMe3 gave resp. the iodo derivs. [(n5-C5H4COONS)Mo(CO)3I] (9) and [(n5-C5H4COONS)Fe(CO)2I] (10) as deep red microcryst. solids. The reactivity of the  $\pi$ -bonded activated ester complexes 5 and 6 and that of the metal-bonded activated ester 7 with amino esters are presented and

ANSWER 7 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

Ι

1995:88027 CAPLUS AN

DN 122:10189

OREF 122:2265a,2268a

discussed.

- Synthesis of the new organometallic carboxylic acid complexes  $[(\eta_5-C5H4COOH)M(CO)nMe]$  (M = Mo, n = 3; M = Fe, n = 2) and their potential as bioconjugates
- ΑU Mouatassim, Bouchra El; ElAmouri, Hani; Salmain, Michele; Jaouen, Gerard CS Ecole Nationale Superieure de Chimie de Paris, 11 rue Pierre et Marie
- Curie, Paris, 75231/05, Fr. SO Journal of Organometallic Chemistry (1994), 479(1-2), C18-C20
- CODEN: JORCAI; ISSN: 0022-328X DT Journal
- LA English
- os CASREACT 122:10189

GI

AB

L3

$$\begin{array}{c} \text{OC} \\ \text{L}_{n} - \text{M} \\ \text{Me} \end{array} \begin{array}{c} \text{O} \\ \text{CO} - \text{N} \end{array}$$

= 2 (5)] were synthesized in 61% and 63% yields, resp., and treated with N-hydroxysuccinimide (HONS) to yield the corresponding activated ester derivs. [( $\eta$ 5-C5H4COONS)M(CO)nMe] [I; M = Mo, n = 3 (3); M = Fe, n = 2, (6)]. The metal-activated ester complex, [( $\eta$ 5-C5H5)Mo(CO)3(CH2COONS)] (8) was obtained similarly, the ester unit being bonded directly to the metal rather than to the  $\pi$ -bonded cyclopentadienyl. The reactivity and potential of the above species as labeling agents for amino acids is discussed.

L3 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

AN 1994:435776 CAPLUS

DN 121:35776

OREF 121:6619a,6622a

TI Novel N-succinimidyl and N-sulfosuccinimidyl organotungsten reagents for the labeling of biological systems

AU Gorfti, Abdellaziz; Salmain, Michele; Jaouen, Gerard

CS Ec. Natl. Super. Chim., Paris, F-75231, Fr.

т

SO Journal of the Chemical Society, Chemical Communications (1994), (4), 433-4

CODEN: JCCCAT; ISSN: 0022-4936

DT Journal LA English

OS CASREACT 121:35776

GI

AB New organotungsten reagents, e.g., I (X = H or SO3Na), bearing a N-succinimidyl or N-sulfosuccinimidyl ester function have been prepared, specifically coupled with amines, amino acids and proteins, and provide a promising basis for the preparation of heavy metal labeling agents designed for x-ray structural anal. of biol. systems.

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FULL ESTIMATED COST 26.00 212.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL





ring nodes:
1 2 3 4 5 7 9 11 12 13 14 15 16 17
ring bonds:
1-2 1-5 1-11 2-3 2-11 3-4 3-7 3-11 4-5 4-11 5-11 7-9 9-14 11-15 12-13
12-17 13-14 14-15 15-16 16-17
exact/norm bonds:

G1:C,Si,Ge

G2:0, S, N, P, As, Sb, Se, Te

G3:Cr, Mo, W

G4:C, N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:Atom

## L1 STRUCTURE UPLOADED

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(FILE 'HOME' ENTERED AT 11:13:59 ON 11 MAY 2009)

FILE 'REGISTRY' ENTERED AT 11:14:10 ON 11 MAY 2009 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS L1 STR



G4 G4

G1 C, Si, Ge G2 O, S, N, P, As, Sb, Se, Te

G3 Cr,Mo,W

G4 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s 11 full FULL SEARCH INITIATED 11:14:57 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 3726 TO ITERATE

100.0% PROCESSED 3726 ITERATIONS SEARCH TIME: 00.00.01 9 ANSWERS

L2 9 SEA SSS FUL L1

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SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST

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FILE COVERS 1907 - 11 May 2009 VOL 150 ISS 20 FILE LAST UPDATED: 8 May 2009 (20090508/ED) REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

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http://www.cas.org/legal/infopolicy.html

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L3
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    ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
    2005:564698 CAPLUS
AN
DN
     143:78676
TΙ
    Monocyclopentadienyl complexes for polymerization of olefins
    Mihan, Shahram; Enders, Markus; Fernandez, Pablo
TN
PA
     Basell Polvolefine G.m.b.H., Germany
SO
     PCT Int. Appl., 66 pp.
     CODEN: PIXXD2
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DT Patent

=> s 12

LA English FAN.CNT 1

										APPLICATION NO.									
PI	WO 2005058983 WO 2005058983			A2				WO 2004-EP14253											
	110	W:	AE, CN, GE,	AG, CO, GH,	AL, CR, GM,	AM, CU, HR,	AT, CZ, HU,	AU, DE, ID, LV,	AZ, DK, IL,	BA, DM, IN,	DZ, IS,	EC, JP,	EE, KE,	EG, KG,	ES, KP,	FI, KR,	GB, KZ,	GD, LC,	
		RW:	TJ, BW,	TM, GH,	TN, GM,	TR, KE,	TT,	PL, TZ, MW, RU,	UA, MZ,	UG, NA,	US, SD,	UZ, SL,	VC, SZ,	VN, TZ,	YU, UG,	ZA, ZM,	ZM,	ZW AM,	
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substituted by at least one bridged donor, where the bridge contains at least one atom of group 14 of the Periodic Table and at least one atom of group 15 or 16 of the Periodic Table, and a catalyst system comprising at least one of the monocyclopentadienyl complexes, and also methods of preparing them, the use of the catalyst system for the polymerization or copolymn.

of olefins and a process for preparing polyolefins by polymerization or copolymn. of

olefins in the presence of the catalyst system and the preparation of the

## associated cyclopentadienyl system.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

TETATO DAME

- AN 2002:157783 CAPLUS
- DN 136:217186
- Catalysts for olefin polymerization and metallocene having bicyclic nitrogen ligands
- IN Andell, Ove; Maaranen, Janne; Hoikka, Jouni; Vanne, Tiina; Rautio, Soile Borealis Technology Oy, Finland; Campbell, Neil

3 DD1 7 03 M7 011 110

- PA PCT Int. Appl., 55 pp. SO
- CODEN: PIXXD2
- DT Patent
- LA English
- FAN.CNT 1

	PATENT NO.				KIND DATE			APPLICATION NO.									
PI	WO 20	020163	74													0010	821
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GT																	

- The title catalysts have ligands I, where LIG = an  $\eta 5$ -ligand AB substituted by a group R1 and a group (R)m; X = 1-3 atom bridge; Y = N or P atom; Z = a C, N or P atom; A1, A2 = optionally substituted heterocyclic ring of 5-12 atoms; R1 = H or other group; R = ring substituent which does not form a  $\sigma$ -bond to a metal  $\eta$ -bonded by the bicyclic ring; m = 0 or 1-3. Co-catalysts selected from aluminoxane or boron compds. are used with the metallocene catalysts. Thus, ethylene was polymerized using triazabicyclodec-ene-yl-1-dimethylsilyl dimethyl-tert-butyldimethylsiloxy dimethylcyclopentadienyl chromium dichloride (preparation given) to give
- polyethylene having m.p. 134.3°. RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL
FULL ESTIMATED COST	7.00	193.58
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY -1.64	SESSION -1.64

STN INTERNATIONAL LOGOFF AT 11:16:02 ON 11 MAY 2009